Algebric Multigrid using Energy-Minimization in Parallel Setting

Andrey Prokopenko

Jeremie Gaidamour, Jonathan Hu, Ray Tuminaro

International Conference On Preconditioning Techniques For Scientific And Industrial Applications

21 June 2013

Sandia National Laboratories

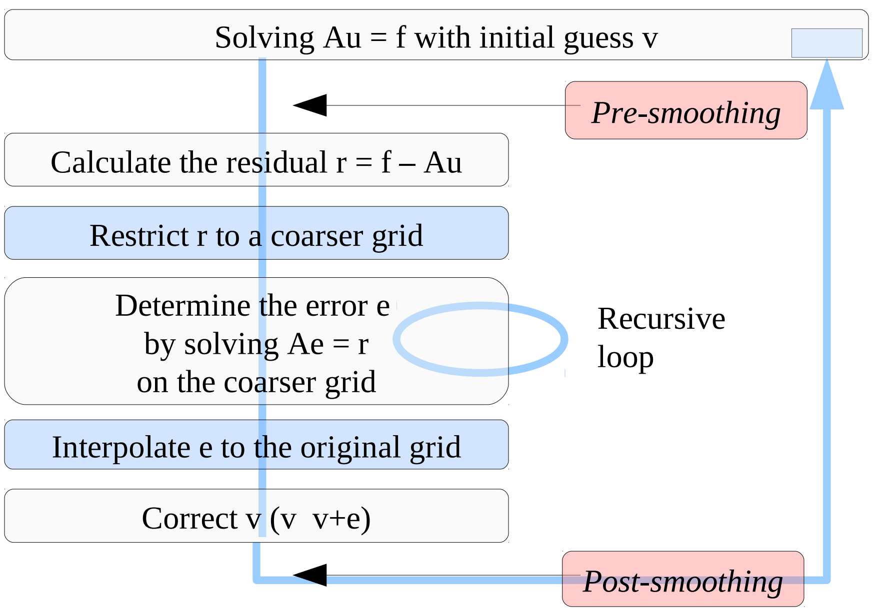
Sandia National Laboratories is a multi-program laboratory operated by Sandia Corp, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

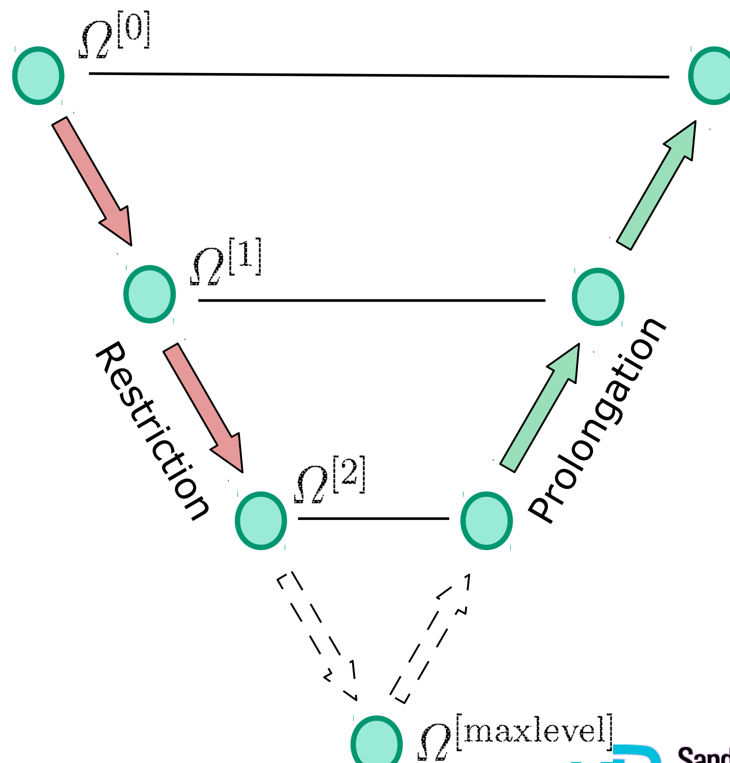
Outline

- Introduction
- Energy-minimization based AMG
  - Motivations
  - Algorithm
- Parallel implementation
- Setup amortization
- Conclusion

AMG

- Iterative method for solving linear equations
- Commonly used as a preconditioner
- Idea: capture error at multiple resolutions using grid transfer operator:
  - **Smoothing** damps the oscillatory error (high energy)
  - **Coarse grid correction** reduces the smooth error (low energy)





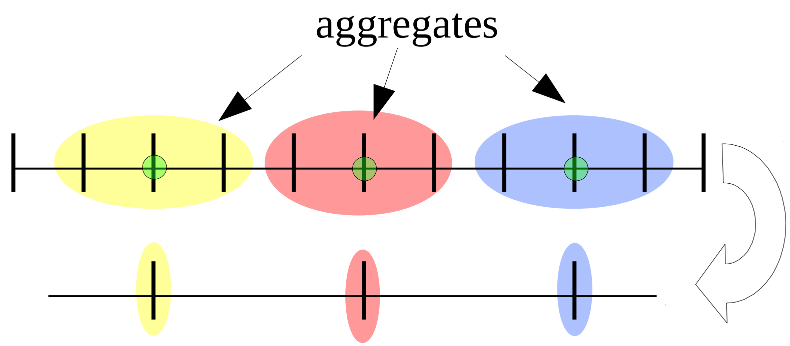
Prolongator requirements

Few desired properties

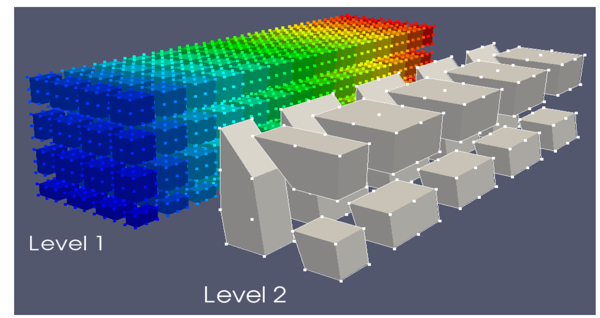
- **preservation of null space**: the span of basis functions on each coarse level should contain zero energy modes
- **minimization of energy**: basis functions on the coarse levels should have as small energy as possible
- **bounded intersection:** the supports of the basis functions on the coarse levels should overlap as little as possible.

Smoothed Aggregation

SA prolongator is constructed in a few steps



- Construct aggregates
  - Select a set of root nodes
  - Group unknowns into aggregates



- Construct tentative prolongator and coarse nullspace
  - Restrict fine nullspace onto aggregates
  - Do QR decomposition

  We satisfy $\mathrm{P}_{tent} B_c = B$

$$B = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ \vdots \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & & \\ 1 & & \\ 1 & & \\ & 1 & \\ & 1 & \cdots \\ & 1 & \\ & & \ddots \end{bmatrix}$$

- Decrease energy of P_{tent} by smoothing

  $\mathrm{P} = (\mathrm{I} - \omega D^{-1} A) P_{tent}$

  May not satisfy $\mathrm{P}_{SA} B_c = B$

Energy minimization

Energy minimization

Energy minimization is a general framework.

Idea: construct the prolongator P by minimizing the energy of each column P_k while enforcing constraints.

Find P:

$$\mathrm{P} = \operatorname{argmin} \sum \|P_k\|_\chi$$

subject to

- specified sparsity pattern;
- nullspace preservation.

Advantages:

- Flexibility (input):
  - accept any sparsity pattern (arbitrary basis function support)
  - enforce constraints: important modes requiring accurate interpolation
  - choice of norm for minimization and search space
- Robustness

Constraint matrix

- Sparsity pattern
- B, B_c fine and coarse mode(s) requiring accurate interpolation

Preservation of the nullspace: for instance $\mathrm{P}1 = 1$

$\left.\right\}$ inputs

$$N = \begin{bmatrix} * & * \\ * & 0 \\ * & * \\ 0 & * \end{bmatrix} \qquad \mathrm{PB}_c = B \Leftrightarrow \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \\ p_{31} & p_{32} \\ p_{41} & p_{42} \end{bmatrix} \begin{bmatrix} b_{11}^c \\ b_{21}^c \end{bmatrix} = \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix}$$

- Representation of the constraints in the algorithm:

$$\mathrm{XP} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ b_{11}^c & 0 & 0 & 0 & b_{21}^c & 0 & 0 & 0 \\ 0 & b_{11}^c & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_{11}^c & 0 & 0 & 0 & b_{21}^c & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_{21}^c \end{bmatrix} \begin{bmatrix} p_{11} \\ p_{21} \\ p_{31} \\ p_{41} \\ p_{12} \\ p_{22} \\ p_{32} \\ p_{42} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix}$$

Constraint matrix

Two nullspace vectors:

$$P \begin{bmatrix} b^c_{11} & b^c_{12} \\ b^c_{21} & b^c_{22} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \\ b_{41} & b_{42} \end{bmatrix}$$

$$\begin{bmatrix} b^c_{11} & 0 & 0 & b^c_{21} & 0 & 0 \\ 0 & b^c_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & b^c_{11} & 0 & b^c_{21} & 0 \\ 0 & 0 & 0 & 0 & 0 & b^c_{21} \\ b^c_{12} & 0 & 0 & b^c_{22} & 0 & 0 \\ 0 & b^c_{12} & 0 & 0 & 0 & 0 \\ 0 & 0 & b^c_{12} & 0 & b^c_{22} & 0 \\ 0 & 0 & 0 & 0 & 0 & b^c_{22} \end{bmatrix} \begin{bmatrix} p_{11} \\ p_{21} \\ p_{31} \\ p_{12} \\ p_{32} \\ p_{42} \end{bmatrix} = \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \\ b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \end{bmatrix}$$

Energy-minimization algorithm

Find P:

$$\mathrm{P} = \operatorname{argmin} \sum \|P_k\|_{\mathcal{X}}$$

subject to

- specified sparsity pattern;
- nullspace preservation.

Solve AP = 0
in a constrained Krylov space

- Definition of energy $\|\cdot\|_{\mathcal{X}}$ depends on Krylov method
  - A for CG
  - $A^T A$ for GMRES

Energy minimization algorithm

Construct aggregates
$\mathcal{N} = |A||P^{(0)}|$ ▷ Select sparsity pattern

$D = diag(A)$ ▷ Diagonal preconditioner
$R = -AP^{(0)}$ ▷ Initial residual
$R = \mathbf{enforce}(R, \mathcal{N})$ ▷ Enforce sparsity on R
$R = \mathbf{project}(R, X)$ ▷ Enforce $RB_c = \mathbf{0}$

for i to iter **do**
$\quad Z = D^{-1}R$
$\quad \gamma =< R, Z >_F$
$\quad$ **if** i is 1 **then**
$\quad\quad Y = Z$
$\quad$ **else**
$\quad\quad \beta = \gamma/\gamma_{old};$
$\quad\quad Y = Z + \beta Y$ ▷ New search direction
$\quad$ **end if**
$\quad \gamma_{old} = \gamma$
$\quad Y_A = AY$
$\quad Y_A = \mathbf{enforce}(Y_A, \mathcal{N})$ ▷ Enforce sparsity on Y_A
$\quad Y_A = \mathbf{project}(Y_A, B_c)$ ▷ Enforce $Y_A B_c = \mathbf{0}$
$\quad \alpha = \gamma / < Y, Y_A >_F$
$\quad P^{(i)} = P^{(i-1)} + \alpha Y$ ▷ Update prolongator
$\quad R = R - \alpha Y_A$ ▷ Update residual

Comparison with Smoothed Aggregation

- SA: 6 DOFs/node
- Energy Minimization: 3 DOFs/node, 6 nullspace vectors

Tab. : Iteration count and *complexity* (lower complexity = faster run time) for increasing mesh sizes and stretch factors.

Mesh	$\epsilon = 1$				$\epsilon = 10$				$\epsilon = 100$			
	SA		Emin		SA		Emin		SA		Emin	
10^3	6	*1.30*	7	*1.07*	8	*2.81*	8	*1.22*	9	*3.21*	8	*1.24*
15^3	8	*1.19*	9	*1.05*	10	*2.32*	10	*1.15*	12	*2.54*	12	*1.16*
20^3	8	*1.24*	9	*1.06*	10	*2.59*	9	*1.18*	13	*3.05*	10	*1.20*
25^3	9	*1.26*	8	*1.07*	11	*2.76*	9	*1.20*	14	*3.04*	10	*1.20*
30^3	10	*1.22*	11	*1.05*	12	*2.52*	12	*1.17*	15	*3.06*	13	*1.19*
35^3	10	*1.24*	10	*1.06*	12	*2.66*	12	*1.18*	16	*3.03*	13	*1.19*
40^3	10	*1.26*	9	*1.06*	12	*2.77*	12	*1.19*	16	*3.21*	11	*1.21*

3.85x

complexity: $$\frac{\sum_i nnz(A_i)}{nnz(A)}$$

Sandia National Laboratories

Parallel implementation

Energy minimization algorithm

Construct aggregates

$\mathcal{N} = |A||P^{(0)}|$ ▷ Select sparsity pattern

$D = diag(A)$ ▷ Diagonal preconditioner

$R = -AP^{(0)}$ ▷ Initial residual

$R = \textbf{enforce}(R, \mathcal{N})$ ▷ Enforce sparsity on R

$R = \textbf{project}(R, X)$ ▷ Enforce $RB_c = \mathbf{0}$

for i to iter **do**

  $Z = D^{-1}R$

  $\gamma =< R, Z >_F$

  if i is 1 **then**

    $Y = Z$

  else

    $\beta = \gamma / \gamma_{old};$

    $Y = Z + \beta Y$ ▷ New search direction

  end if

  $\gamma_{old} = \gamma$

  $Y_A = AY$

  $Y_A = \textbf{enforce}(Y_A, \mathcal{N})$ ▷ Enforce sparsity on Y_A

  $Y_A = \textbf{project}(Y_A, B_c)$ ▷ Enforce $Y_A B_c = \mathbf{0}$

  $\alpha = \gamma / < Y, Y_A >_F$

  $P^{(i)} = P^{(i-1)} + \alpha Y$ ▷ Update prolongator

  $R = R - \alpha Y_A$ ▷ Update residual

Energy minimization algorithm

Construct aggregates
$\mathcal{N} = |A||P^{(0)}|$ ▷ Select sparsity pattern

$D = diag(A)$ ▷ Diagonal preconditioner
$R = -AP^{(0)}$ ▷ Initial residual
$R = \mathbf{enforce}(R, \mathcal{N})$ ▷ Enforce sparsity on R
$R = \mathbf{project}(R, X)$ ▷ Enforce $RB_c = \mathbf{0}$

for i to iter **do**
    $Z = D^{-1}R$
    $\gamma = < R, Z >_F$
    if i is 1 **then**
        $Y = Z$
    else
        $\beta = \gamma / \gamma_{old};$
        $Y = Z + \beta Y$ ▷ New search direction
    end if
    $\gamma_{old} = \gamma$
    $Y_A = AY$
    $Y_A = \mathbf{enforce}(Y_A, \mathcal{N})$ ▷ Enforce sparsity on Y_A
    $Y_A = \mathbf{project}(Y_A, B_c)$ ▷ Enforce $Y_A B_c = \mathbf{0}$
    $\alpha = \gamma / < Y, Y_A >_F$
    $P^{(i)} = P^{(i-1)} + \alpha Y$ ▷ Update prolongator
    $R = R - \alpha Y_A$ ▷ Update residual

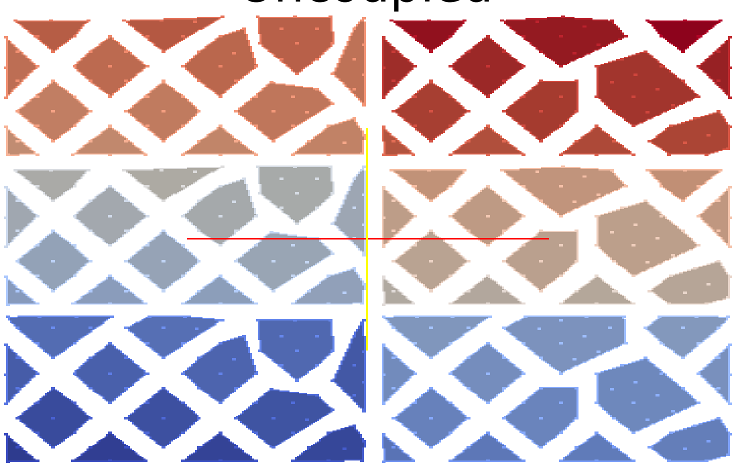
Sandia National Laboratories

Parallel aggregation

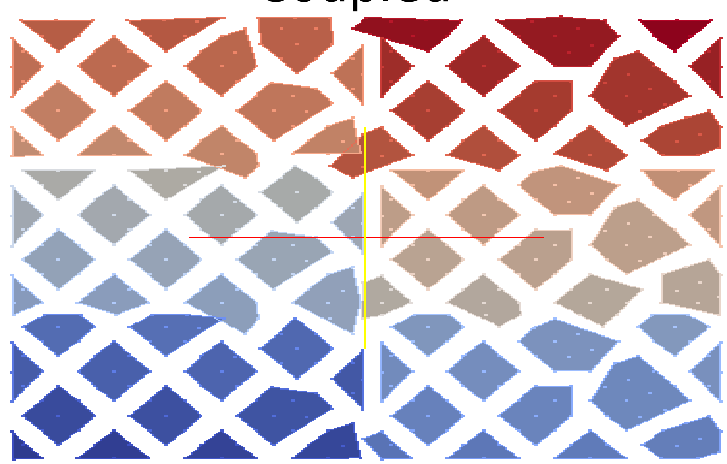
Two choices: coupled and uncoupled aggregation

- Uncoupled aggregation aggregates only inside a subdomain
- Coupled aggregation allows aggregates to cross subdomain boundary
- Coupled aggregation is more expensive, but has convergence similar to the serial case

Uncoupled



Coupled



Constraints in parallel

Let P have the following pattern and nullspace consist of two vectors

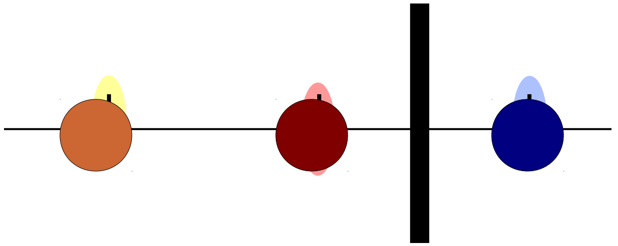
$$P \begin{bmatrix} b^c_{11} & b^c_{12} \\ b^c_{21} & b^c_{22} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \\ b_{41} & b_{42} \end{bmatrix} \qquad P = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & 0 \\ p_{31} & p_{32} \\ 0 & p_{41} \end{bmatrix}$$

$$\begin{bmatrix} b^c_{11} & 0 & 0 & b^c_{21} & 0 & 0 \\ 0 & b^c_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & b^c_{11} & 0 & b^c_{21} & 0 \\ 0 & 0 & 0 & 0 & 0 & b^c_{21} \\ b^c_{12} & 0 & 0 & b^c_{22} & 0 & 0 \\ 0 & b^c_{12} & 0 & 0 & 0 & 0 \\ 0 & 0 & b^c_{12} & 0 & b^c_{22} & 0 \\ 0 & 0 & 0 & 0 & 0 & b^c_{22} \end{bmatrix} \begin{bmatrix} p_{11} \\ p_{21} \\ p_{31} \\ p_{12} \\ p_{32} \\ p_{42} \end{bmatrix} = \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \\ b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \end{bmatrix}$$

$$\begin{bmatrix} b^c_{11} & b^c_{21} & 0 & 0 & 0 & 0 \\ b^c_{12} & b^c_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & b^c_{11} & 0 & 0 & 0 \\ 0 & 0 & b^c_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & b^c_{11} & b^c_{21} & 0 \\ 0 & 0 & 0 & b^c_{12} & b^c_{22} & 0 \\ 0 & 0 & 0 & 0 & 0 & b^c_{21} \\ 0 & 0 & 0 & 0 & 0 & b^c_{22} \end{bmatrix} \begin{bmatrix} p_{11} \\ p_{12} \\ p_{21} \\ p_{32} \\ p_{41} \\ p_{42} \end{bmatrix} = \begin{bmatrix} b_{11} \\ b_{12} \\ b_{21} \\ b_{22} \\ b_{31} \\ b_{32} \\ b_{41} \\ b_{42} \end{bmatrix}$$

Constraints in parallel

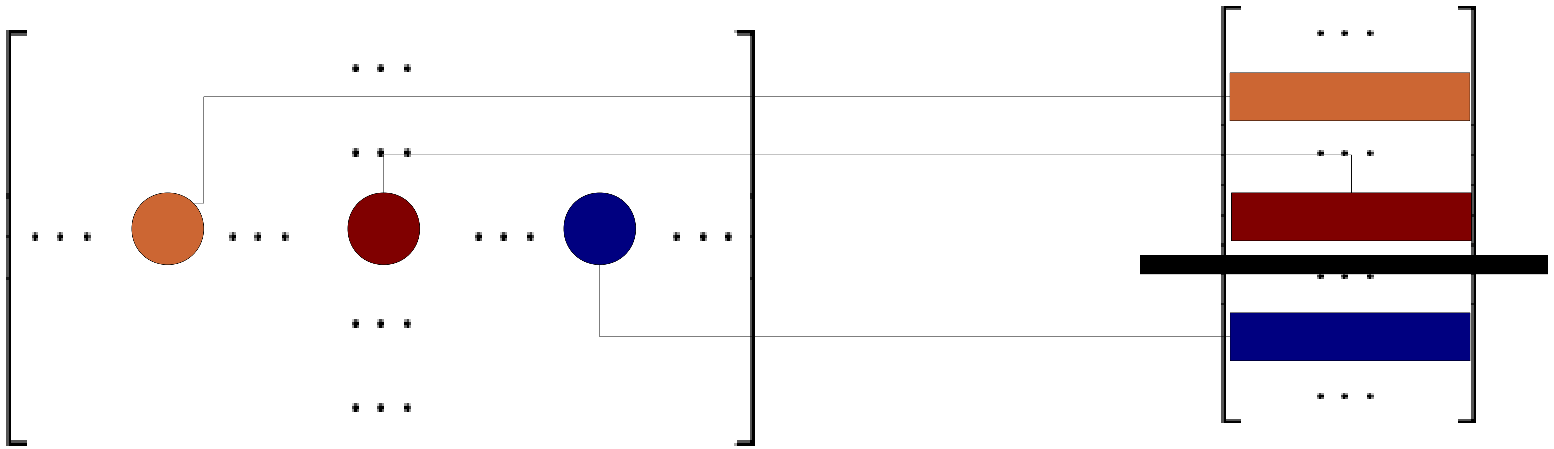
What does each block correspond to?



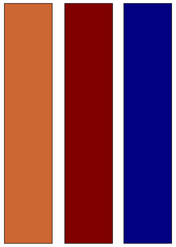
Consider a row of P with three nonzeros

Prolongator row

Coarse nullspace



Block of the constraint corresponding to the row



Energy minimization algorithm (updated)

Construct aggregates

$\mathcal{N} = |A||P^{(0)}|$ ▷ Select sparsity pattern

Import ghost components of nullspace vectors

$D = diag(A)$ ▷ Diagonal preconditioner

$R = -AP^{(0)}$ ▷ Initial residual

$R = \textbf{enforce}(R, \mathcal{N})$ ▷ Enforce sparsity on R

$R = \textbf{project}(R, X)$ ▷ Enforce $RB_c = \mathbf{0}$

for i to iter **do**

$Z = D^{-1}R$

$\gamma =< R, Z >_F$

if i is 1 **then**

$Y = Z$

else

$\beta = \gamma/\gamma_{old};$

$Y = Z + \beta Y$ ▷ New search direction

end if

$\gamma_{old} = \gamma$

$Y_A = AY$

$Y_A = \textbf{enforce}(Y_A, \mathcal{N})$ ▷ Enforce sparsity on Y_A

$Y_A = \textbf{project}(Y_A, B_c)$ ▷ Enforce $Y_A B_c = \mathbf{0}$

$\alpha = \gamma / < Y, Y_A >_F$

$P^{(i)} = P^{(i-1)} + \alpha Y$ ▷ Update prolongator

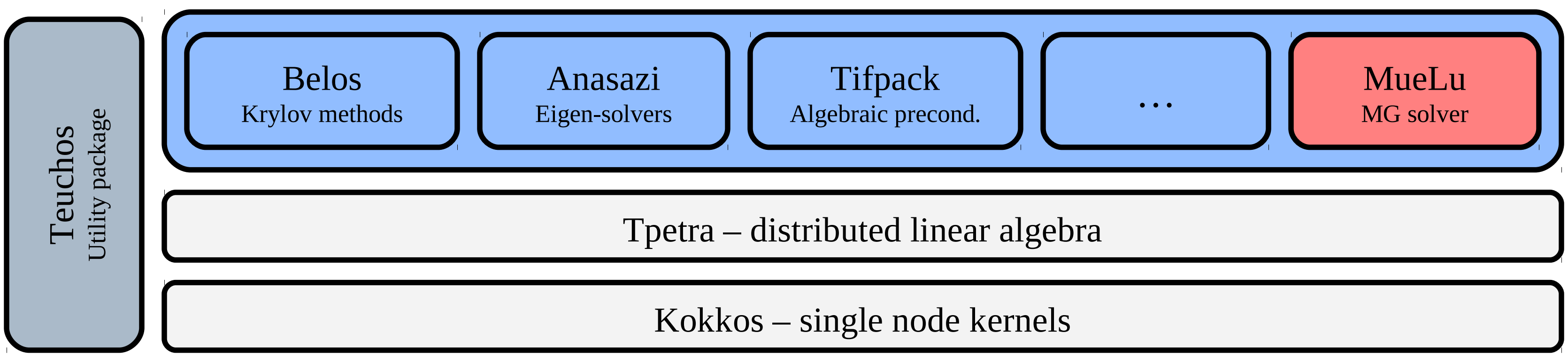
$R = R - \alpha Y_A$ ▷ Update residual

MueLu

- Future package of the Trilinos project (to replace ML)
  - Massively parallel
  - Multicore and GPU aware
  - Templated types for mixed precision calculation (32-bit – 64-bit) and type complex

- Objective is to solve problem with billions of DOF on 100Ks of cores…

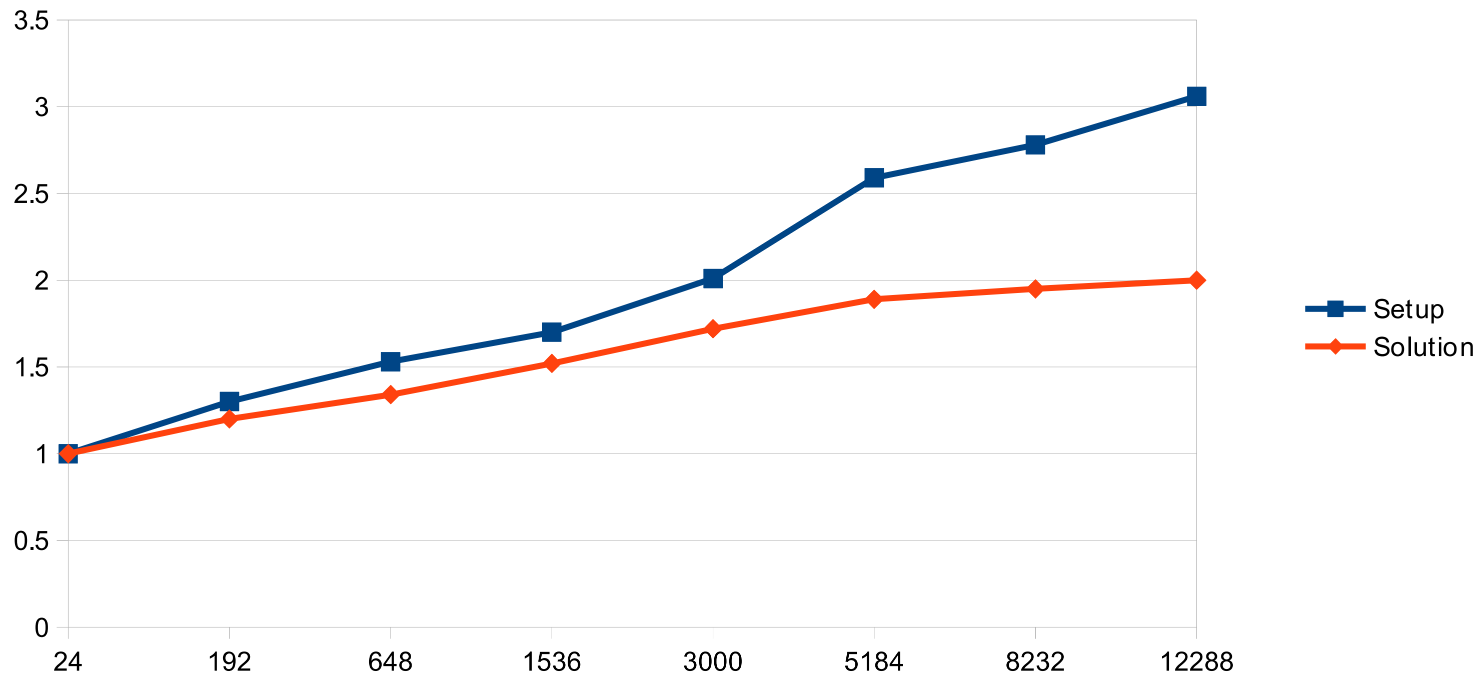
- Leverage the Trilinos software stack:



- Currently in development…

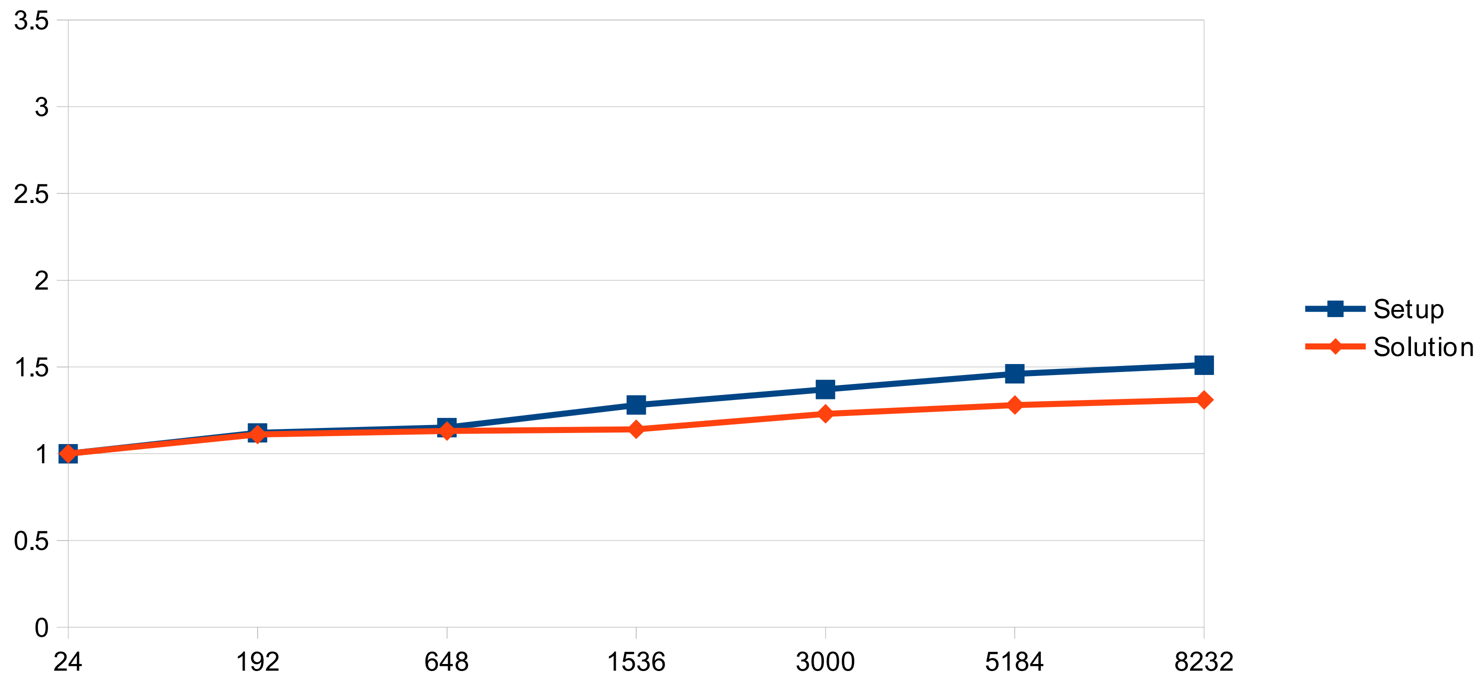
Numerical results – Laplace 3D

- Laplace 3D, 7 point stencil
- Energy minimization
  - 2 CG iterations
  - Initial guess: tentative prolongator
  - Sparsity pattern: same as SA



Numerical results – Elasticity 3D

- Elasticity 3D, Poisson ratio 0.25
- Energy minimization
  - 2 CG iterations
  - Initial guess: tentative prolongator
  - Sparsity pattern: same as SA



Setup amortization

Setup amortization: reuse

- Emin setup may be expensive (several times that of SA)

- Typically, we need multigrid for each linear iteration of Newton, therefore it is reasonable to assume that the system does not change too much

- Many components of the setup phase can be reused
  - Initial prolongator
  - Sparsity patterns (assuming no filtering)
  - Matrix graphs (assuming fixed mesh)

Strategies for a sequence of systems

- **No reuse**: construct multigrid anew for each iteration
- **Simple reuse**: construct multigrid only for the first iteration, and then use the same preconditioner for all iteration
- **Fast reuse**: construct multigrid with multiple iterations on the first step, and use fewer iterations for consecutive step, reusing constructed prolongators and graphs

Numerical example: icesheet model

System of two coupled non-linear PDEs

$$\begin{cases} -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_1) & = & -\rho g \frac{\partial s}{\partial x}, \\ -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_2) & = & -\rho g \frac{\partial s}{\partial y} \end{cases}$$

with Glen's law viscosity

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\dot{\epsilon}_{xx}^2 + \dot{\epsilon}_{yy}^2 + \dot{\epsilon}_{xx}\dot{\epsilon}_{yy} + \dot{\epsilon}_{xy}^2 + \dot{\epsilon}_{xz}^2 + \dot{\epsilon}_{yz}^2 + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

$$\dot{\boldsymbol{\epsilon}}_1^T = \left(\; 2\dot{\epsilon}_{xx} + \dot{\epsilon}_{yy}, \quad \dot{\epsilon}_{xy}, \quad \dot{\epsilon}_{xz} \; \right)$$

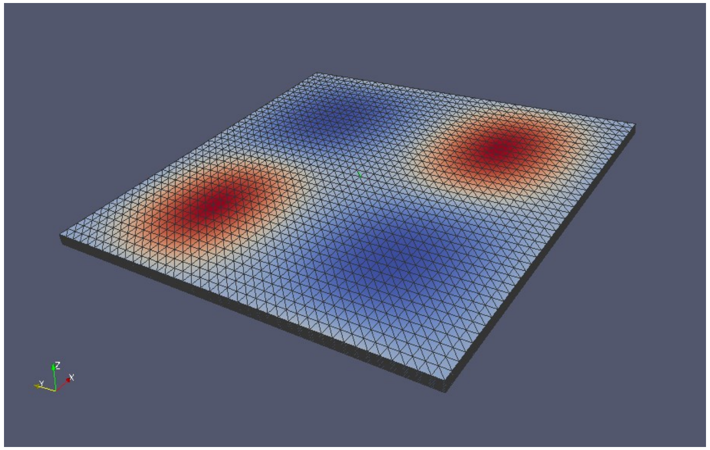
$$\dot{\boldsymbol{\epsilon}}_2^T = \left(\; \dot{\epsilon}_{xy}, \quad \dot{\epsilon}_{xx} + 2\dot{\epsilon}_{yy}, \quad \dot{\epsilon}_{yz} \; \right)$$

$$\dot{\epsilon}_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

$$\begin{array}{lcl} A & = & \text{flow rate factor} \\ n & = & \text{Glen's law exponent} = 3 \\ \gamma & = & \text{regularization parameter} \\ \beta & = & \text{sliding coefficient} \geq 0 \end{array}$$

Discretization: classical Galerkin FEM with structured or unstructured mesh.

Nonlinear solver: Newton's method



Sandia National Laboratories

Numerical results: icesheet model

Step	Emin(6)	Emin(1)	Emin(6,1)
2	17	30	17
8	16	32	17
12	17	33	18
18	17	36	18
23	17	36	18
28	17	34	18

Sandia National Laboratories

Summary

- Energy minimization AMG is flexible
- Energy minimization AMG is suitable for parallelization
  - Standard parallel operations (MxM, BLAS1) are well known
  - Constraint application could be done locally storing ghost info
- Preliminary results show promise
- There are ways to reduce setup cost